*ANALYSIS OF SULFUR HETEROCYCLES IN COAL-DERIVED PRODUCTS AND SHALE OILS** C. Willey M. Iwao, T. A. Broadbent, R. N. Castle, and M. L. Lee, Department of Chemistry, Brigham Young University, Provo, Utah 84602.

The carcinogenic activity demonstrated by complex mixtures of polycyclic aromatic compounds (PAC) has stimulated much effort by researchers to identify individual mixture components. Found in low concentrations among the mixture components of most PAC fractions from coal-derived products and shale oils are the sulfur heterocycles. Due to their low concentrations, an enrichment of the heterocyclic sulfur compounds is necessary for identification. A recently developed method to isolate the sulfur heterocycle fraction from a composite aromatic fraction has greatly aided efforts to separate and identify individual heterocyclic sulfur compounds by glass capillary gas chromatographic mass spectrometry.

In this study, the developed methodology for the enrichment and subsequent separation and identification of sulfur heterocycle fractions has been applied to selected coal gasification tars, coal liquids, and shale oils. Identification was accomplished through comparison of mass spectral and chromatographic retention data of mixture components with standard reference compounds.

Since few standard reference compounds of sulfur heterocycles are commercially available, compounds predicted by mass spectrometry to be present in enriched sulfur heterocycle fractions were synthesized. These compounds were used to obtain chromatographic retention data and for biological testing.

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